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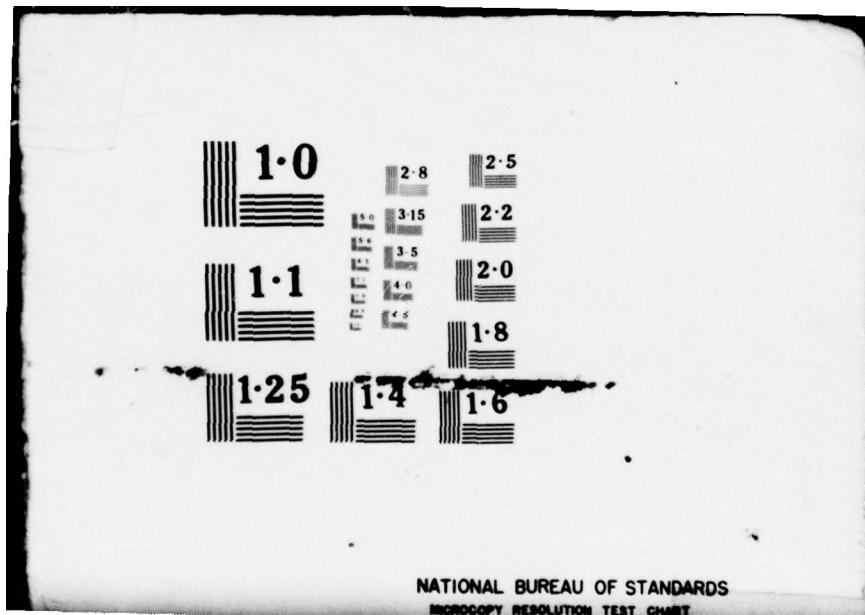
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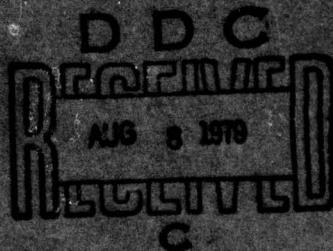
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For the period April 1, 1978 through March 31, 1979

JOINT SERVICES ELECTRONICS PROGRAM

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ELECTRONICS RESEARCH CENTER

The University of Texas at Austin

Austin, Texas 78712

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The Electronics Research Center at The University of Texas at Austin consists of interdisciplinary laboratories in which graduate faculty members and graduate candidates from numerous academic disciplines conduct research. The disciplines represented in this report include information electronics, solid state electronics and quantum electronics.

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10 Submitted by Edward J. Powers
on behalf of the faculty and staff
of the Electronics Research Center

Technical Editor: Steven I. Marcus

11 15 July 15, 1979

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ABSTRACT

This report summarizes progress on projects carried out at the Electronics Research Center at The University of Texas at Austin and which were supported by the Joint Services Electronics Program. In the area of Information Electronics progress is reported for projects involving (1) nonlinear filtering and estimation, (2) electronic multi-dimensional signal processing, (3) electronic control systems, (4) electronic computer system design and analysis and (5) electronic computer software systems.

In the Solid State Electronics area recent findings in (1) basic solid state materials research and (2) research on instabilities and transport near surfaces and interfaces of solids are described.

In the area of Quantum Electronics progress is presented for the following projects: (1) nonlinear wave phenomena, (2) atomic and molecular electronic processes and (3) high power laser systems.

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Advanced Degrees Awarded

*John Beall, EE, M.S., May 1979, "Digital Bispectral Analysis of Nonlinear Effects in an RF-Excited Glow Discharge Plasma"

H. Nelson Brady, EE, M.S., December 1978, "The Use of Microprocessors in Controlling Dynamic Multiple-Connected Subsystems"

Hsien-Ching K. Chen, EE, M.S., May 1978, "Banyan Network Logic Design and Hardware Construction"

Mark Chonko, EE, M.S., May 1979, "A Feedback Controlled System for the Precise Measurement of Weak Current-Voltage Non-Linearities"

Manuel d'Abreu, EE, Ph.D., December 1978, "Analysis and Synthesis of Data Structures and Algorithms for an Accurate Functional Level Concurrent Fault Simulator"

Jae Y. Hong, EE, M.S., May 1979, "Development of a Plasma Fluctuation Diagnostic Based on Digital Time Series Analysis"

James Cheng Hu, EE, M.S., August 1978, "A Study of the Sili-cides Formation for Thin Cobalt Film on Single Crystal Silicon"

Patrick G. Karger, EE, M.S., August 1978, "Automatic Modularization of Gate Level Networks to Facilitate the Simulation of Large Digital Systems"

Young C. Kim, EE, Ph.D., August 1978, "Digital Bispectral Analysis and Its Application"

*Denotes students who have contributed to JSEP projects, but who have not been paid out of JSEP funds (e.g., students on fellowships).

PERSONNEL AND RESEARCH AREAS

Advanced Degrees Awarded (Cont.)

Rafael Lemus, EE, M.S., May 1979, "Synchronization of Concurrent Transactions in a Distributed Database Management System"

Chang-Huan Liu, EE, M.S., August 1978, "A Comparison of Optimal and Suboptimal Estimators and Estimation Lower Bounds"

Dariush Minoo-Hamedani, EE, M.S., August 1978, "Mean Square Prediction Using a Memoryless Nonlinearity Followed by a Linear Filter"

Hao Nhi Nham, EE, M.S., May 1978, "Design and Implementation of a Cost-Effective Digital Logic Test-Generation System"

Ernesto Pacas-Skewes, EE, Ph.D., May 1979, "A Design Methodology for Digital Systems Using Petri Nets"

William Russell Read, Jr., EE, M.S., May 1978, "Hierarchical Methods for Generating Tests for Sequential Logic Networks in a Simulation Environment"

John W. Smith II, EE, M.S., August 1978, "Automatic Generation of Evaluation Routines for Modular Level Simulation"

Michael M.H. Tong, EE, M.S., May 1979, "Crash Recovery in Distributed Systems"

*Randall O. Withrow, EE, M.S., May 1979, "A Digital Data Acquisition System Used in the Determination of the Spectral Index of Turbulent Fluctuation Data"

Wai-Fan Wong, EE, M.S., August 1978, "Quadratically Nonlinear Least-Mean-Square Filter"

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- * K.H. Hong, M.H. Proffitt and L.W. Frommhold, "Absolute Cross Sections for Collision-Induced Depolarized Scattering of Light in Krypton and Xenon," *Molec. Phys.* 35, pp. 691-700, 1978.
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*J.P. Stark, "Evolution of Two Phase Dispersion of Volume Diffusion," J. Appl. Phys., in press.

T.K.M. Agerwala, "Communication and Control Issues in Distributed Systems," submitted for publication.

*C. Liu and S.I. Marcus, "Estimator Performance for a Class of Nonlinear Estimation Problems," to appear in IEEE Transactions on Automatic Control.

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*M.H. Proffitt and L. Frommhold, "Collision-Induced Polarized and Depolarized Spectra of Helium and the Diatom Polarizability," to appear in *J. Chem. Phys.*

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*R. Remke, R.M. Walser, and R.W. Bene', "Transition Layers Between CVD- VO_2 and Oxide Substrates," submitted to *Thin Solid Films*.

*J.W. Keto, T.D. Raymond, and S.T. Walsh, "A Low Inductance Spark Gap Switch for Blumlein Driven Lasers," submitted to *Rev. Sci. Inst.*

*J.W. Keto and Chien-Yu Kuo, "Collisional Quenching of A_2^4 (3p) 4 4p and A_2^4 (3p) 3 3d in Electron Beam Excited Argon at High Densities," in preparation.

*R.M. Walser and M.F. Becker, "Preemption of Semiconducting Metallic Phase Transition in VO_2 by Fast, Selective Optical Excitation," to be submitted to *Solid State Comm.*

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A.B. Buckman and A.C. Kwok, "Diffraction from Photolysis Induced Dielectric Gratings in Thin PbI_2 Films," *Journal of the Optical Society of America*, in preparation.

Chien-Yu Kuo and J.W. Keto, "Dissociative Recombination of Ions in Electron Beam Excited Argon at High Densities," in preparation.

*C.F. Hirt, Chien-Yu Kuo, and J.W. Keto, "Production of $\text{O}^1(\text{s}_0)$ in Mixtures of O_2 in Argon Excited by an Electron Beam," in preparation.

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PUBLICATIONS, TECHNICAL PRESENTATIONS, LECTURES AND REPORTS

TECHNICAL PRESENTATIONS AND LECTURES

1978 IEEE International Conference
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Processing
Tulsa, Oklahoma
April 10-12, 1978

*H. Chang and J.K. Aggarwal, "Design of Semi-causal Two-Dimensional Recursive Filters."

IEEE Region V Annual Conference
Tulsa, Oklahoma
April 16-18, 1978

*B.F. Womack and H.W. Lo, "Synthesis of Feedback
Systems with Nonlinear Uncertain Plants."

Solid State Devices, Inc.
Engineering Group
Los Angeles, California
April 19, 1978

R.W. Bene', "Schottky Barriers on Silicon
Surfaces."

Target Modulated Signature Meeting
U.S. Air Force Avionics Laboratory
Wright Patterson Air Force Base, Ohio
April 20, 1978

*E.J. Powers, "Bispectral Analysis of Radar
Data from Vibrating Targets."

1978 IEEE International Conference
on Plasma Science
Monterey, California
May 15-17, 1978

*Y.C. Kim and E.J. Powers, "Application of
Digital Complex Demodulation Techniques in
Analyzing Nonlinear Wave Data."

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PUBLICATIONS, TECHNICAL PRESENTATIONS, LECTURES AND REPORTS

1978 IEEE International Conference
on Plasma Science
(continued)

J.R. Roth, W.M. Krawczonk, E.J. Powers,
J.Y. Hong, and Y.C. Kim, "Functional Dependence
of Radial Transport in a Toroidal Plasma Sub-
ject to Strong Radial Electric Fields."

1978 IEEE International Symposium on
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New York, N.Y.
May 17-19, 1978

*K. Hirano and J.K. Aggarwal, "Design of Two-
Dimensional Recursive Digital Filters with
Half-Plane Symmetry Characteristics."

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Plasma Diagnostics
Monterey, California
May 17-19, 1978

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on Digital Time Series Analysis."

Topical Meeting on Picosecond
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Hilton Head, South Carolina
May 25, 1978

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Detroit, MI
June 2, 1978

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and Applications of Microcomputers."

PUBLICATIONS, TECHNICAL PRESENTATIONS, LECTURES AND REPORTS

IBM
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Yorktown Heights, N.Y.
June 12, 1978

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E.J. Powers, J.Y. Hong, Y.C. Kim, J.R. Roth,
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R.T. Yeh, Current Trends in Programming Methodology: Vol.4 - Data Structuring, Prentice-Hall, June 1978.

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CONSULTATIVE AND ADVISORY FUNCTIONS

M. Becker, L. Frommhold, J. Keto, and E. Powers met with Col. Dale Neal of the Air Force Weapons Laboratory at The University of Texas at Austin, on April 12, 1978, for the purposes of discussing "Laser Beam Control Systems and Adaptive Optics."

A.B. Buckman participated in the Workshop on Applications of Integrated Optics to Missile Guidance, Redstone Arsenal, Huntsville, Alabama, April 18-19, 1978. This meeting was sponsored by the U.S. Army Missile Research and Development Command, and by the U.S. Army Research Office.

E.J. Powers presented the paper "Bispectral Analysis of Radar Data from Vibrating Targets," at the Target Modulated Signature Meeting held at the U.S. Air Force Avionics Laboratory, Wright Patterson Air Force Base, Ohio, April 20, 1978.

E.J. Powers visited Dr. B.H. Ripin at the Naval Research Laboratory on May 9, 1978 for the purposes of discussing diagnostic problems relating to Laser-Fusion Studies at NRL.

Baxter F. Womack visited the Tactical Systems Division, Headquarters, USAF, Pentagon, on August 15, 1978 for the purpose of discussing current and proposed research in commander-decision processes with Dr. D.K. Leedom and Major Howard Anderson.

Jack S. Turner participated in a study of the deflagration to detonation transition in liquid propellants in collaboration with personnel at ARRADCOM (Dover, NJ). The study involved computer modelling of random effects on the DDT transition, and was supported in part by the Scientific Services Program (Contract DAAG29-76-d-0100, D.O. No. 0802) administered by Battelle Columbus Laboratories, Ohio. Consultation visits to ARRADCOM-Dover were made May 2-4 and June 22-23, 1978, and a final report, entitled "Nondeterministic Origins of Detonation in Energetic Media: Random Initiation and Transition in Liquid Propellants," was submitted in November 1978.

G.L. Wise visited with Dr. Joel Morris of the Naval Research Laboratory on March 28, 1979 and discussed some recent research results in signal detection.

I. INFORMATION ELECTRONICS

INFORMATION ELECTRONICS

Research Unit IE8-1. NONLINEAR FILTERING AND ESTIMATION

Principal Investigators: Professor S.I. Marcus (471-3265)
Professor T.J. Wagner (471-3183)
Professor G.L. Wise (471-3356)

Research Associate: Dr. L.P. Devroye

Graduate Students: N. Bagherzadeh, D. Halverson, K. Hsu, C. Liu, and D. Minoo-Hamedani

A. PROGRESS: Historically, significant results in the area of nonlinear systems with random inputs have come forth sparingly and in a sporadic manner. Nevertheless, nonlinear systems are attractive in their promise of increased performance capabilities. This research program was oriented toward the investigation of certain statistical aspects of some forms of nonlinear systems. Specifically, the design and analysis of nonlinear estimators, the design of a nonlinear system for signal detection in dependent non-Gaussian noise, the stochastic stability of systems with multiplicative state noise, and the convergence of non-parametric estimation procedures have been investigated. A more detailed description of this progress follows.

Nonlinear Estimation: The problem of nonlinear state estimation involves the extraction of information about the state of a stochastic system from nonlinear noisy measurements. This is accomplished by passing the measurements through a nonlinear filter, the output of which is the state estimate. The particular objective of this research has been the design, analysis, and implementation of high-performance optimal and suboptimal estimators which operate recursively in real time.

As is well known, it is not possible in general to recursively generate the optimal minimum variance estimate (the conditional mean) of the state of a nonlinear stochastic system, given the past observations, for this would require the recursive computation of the entire conditional density. However in [1] and [2] we have investigated the state estimation problem for certain special classes of nonlinear stochastic systems, described either by Volterra series expansions or by bilinear differential equations with a particular Lie algebraic structure. For these classes of systems, in both continuous and discrete time, we have shown that the optimal conditional mean estimator is recursive and of fixed finite dimension; we have also shown how the estimator can be imple-

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mented on-line in real time. These results represent virtually the only known finite dimensional optimal nonlinear estimators for systems in which both the state and observations are corrupted by Gaussian white noise. The discrete time estimators of [2] display the interesting phenomenon of containing polynomials in the innovations process; this result concerning the structure of optimal discrete time estimators has potential significance in the design of suboptimal discrete time estimators.

Recent results in martingale theory have been applied to discrete time nonlinear recursive estimation problems in [3]; the observations are assumed to take values in a countable space. General methods for constructing system models and deriving optimal estimators are presented, and previously obtained estimation equations are exhibited as special cases. Real time recursive estimators are derived and constructed for systems in which the state is a finite state Markov process.

Also, an investigation of a discrete time nonlinear Wiener filter was begun. The filter was constrained to be composed of a memoryless nonlinearity followed by a linear filter. The study was concerned with determining how to specify the memoryless nonlinearity. Once the nonlinearity is known, the linear filter can be determined with standard techniques. The results of this effort are given in [4] and [5], where several methods for determining the nonlinear system are investigated. It is shown that in many cases a nonlinear system of this form can significantly outperform the optimal linear system.

The investigation of nonlinear estimators is continuing. The research in this area was complemented by the Grant ENG 76-11106 from the National Science Foundation and by the Grant AFOSR-76-3062 from the Air Force Office of Scientific Research.

Signal Detection: The objective of the work in signal detection was the design of a discrete time detector to detect a signal in dependent non-Gaussian noise. That is, a sequence of observations is taken, y_1, y_2, \dots, y_n . If the signal is present, the i -th observation is given by $y_i = s_i + N_i$, for all i , and if the signal is absent, it is given by $y_i = N_i$, where $\{s_i\}$ represents the signal and $\{N_i\}$ represents the noise. From a knowledge of y_1, y_2, \dots, y_n , it is desired to announce whether or not a signal is present. Historically, much work in this area assumes either that the noise is a Gaussian process or that the noise observations are mutually independent.

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However, frequently the noise is non-Gaussian and frequently the waveform is sampled at such a high rate that the independence assumption is invalid.

It is known that if the noise is independent, then the best detection strategy, for a wide variety of performance criteria, is to form the statistic

$$t = \sum_{i=1}^n g_i(y_i) ,$$

where $g_i(\cdot)$ is a function determined by the probability density function of the noise, and then compare this statistic to a threshold, which is selected by the performance specifications of the detection system. If the threshold is exceeded, it is announced that the signal is present. This detection system is easily implemented by use of a memoryless nonlinearity, an accumulator, and a threshold comparator.

If the noise sequence is not independent, then in general a much more complicated statistic must be formulated. Unfortunately, the structure of this statistic is determined by the n -dimensional distribution of the noise, which is rarely known in practical situations.

The approach taken in this research was to constrain the structure of the detection system to be that which results when the noise is independent (i.e. memoryless nonlinearity, accumulator, threshold comparator) and then to account for the dependency in the noise by appropriately choosing the memoryless nonlinearity. The asymptotic performance (i.e. as n becomes large) of the detector was then optimized. Such optimization required only the bivariate density of the noise, as opposed to the n -dimensional density as mentioned above. The noise was modeled as a ϕ -mixing process. Such processes require a "decrease" in dependency as samples are more widely separated in time, but the rate of decrease may be reasonably arbitrary, and thus a great amount of flexibility for modeling is available. Results of this investigation are given in [6] and [7].

The investigation of signal detection is being continued. The research in this area was complemented by the Grant AFOSR-76-3062 from the Air Force Office of Scientific Research.

Stochastic Stability: The objective of the work in stochastic stability was a tractable method to determine the stochastic stability of linear systems with multiplicative noise, that is, systems described by equations of the form

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$$\dot{X}(t) = \left[A + \sum_{i=1}^n B_i f_i(t) \right] X(t)$$

where the $f_i(t)$ are random processes. Notice that the noise is multiplicative instead of additive, accounting for the nonlinear structure of the system. Such systems are popular models for many practical problems, such as circuits with random parameters and the effect of switching jitter on sampled data system performance. In the case that the noise processes are jump processes, such models find application in modeling faulty systems, or systems subject to abrupt random changes. A major concern is the stability of such systems. The objective of this work was the establishment of useful methods for determining when the statistical moments of the state components tend to zero.

A new method for investigating the stochastic stability of the above form of system was introduced. It is based upon the use of the characteristic functional of a random process. That is, if $X(t)$ is a random process, its characteristic functional is given by

$$\phi_X(u) = E\{\exp[i \int X(t)u(dt)]\},$$

where u is a suitably restricted generalized measure. It was shown that for certain types of bilinear systems, the characteristic functional afforded a convenient method for investigation of stochastic stability. In particular, this method was particularly appropriate for situations where the noise processes were filtered Poisson processes. This form of noise provides a good model for a wide variety of phenomena such as shot noise, ELF and VLF atmospheric noises, and other random sporadic events such as the noise generated by a faulty component. The results of this research are given in [8], where several examples are presented.

The investigation of stochastic stability is being continued. The research in this area was complemented by the Grant ENG 76-11106 from the National Science Foundation.

Nonparametric Estimation: In the usual estimation problem one observes a random vector X and wants to estimate the random variable θ . If the joint distribution of (X, θ) is known, then taking $\hat{\theta}$, the estimate of θ , as $E(\theta|X)$, the conditional expectation of θ given X , is the usual choice in that the mean-squared-error of the estimate is minimized.

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If knowledge of the joint distribution of (X, θ) is replaced by data $(X_1, \theta_1), \dots, (X_n, \theta_n)$, a sample of size n drawn from the distribution of (X, θ) , then one has the nonparametric estimation problem where the estimate $\hat{\theta}$ now is a function of both X and the data. If $L = E\{\theta - E(\theta | X)\}^2$ denotes the mean-squared-error for the best estimate of θ when the distribution of (X, θ) is known and if $L_n = E\{(\theta - \hat{\theta})^2 | (X_1, \theta_1), \dots, (X_n, \theta_n)\}$ denotes the mean-squared-error of the nonparametric estimate $\hat{\theta}$ given the data, then we were interested in when and how L_n converged to L as n tends to ∞ assuming only that $E\{\theta^2\} < \infty$.

If K is a bounded Borel function defined on \mathbb{R}^d (d is the dimension of X), and if h_n is a sequence of positive numbers, then

$$\hat{\theta}_n = \sum_{i=1}^n \theta_i K((X_i - X)/h_n) / \sum_{i=1}^n K((X_i - X)/h_n)$$

is the kernel estimate of θ . In [9], mild conditions on K and h_n were given which insure that

$$L_n \xrightarrow{n} L \text{ in probability.} \quad (1)$$

This result nicely complements the first result of this type for nearest neighbor estimates due to Stone [10]. If one replaces the kernel estimate by

$$\hat{\theta}_n = \sum_{i=1}^n \theta_i K((X_i - X)/h_i) / \sum_{i=1}^n K((X_i - X)/h_i)$$

then this new estimate has a recursive flavor if one fixes X and the data unfolds in n . In this case, only the sums

$$\sum_{i=1}^n \theta_i K((X - X_i)/h_i) \text{ and } \sum_{i=1}^n K((X - X_i)/h_i)$$

need to be updated as n

increases, thus eliminating the need for storing the data. (It should be noted, however, that one is no longer treating the data symmetrically.) The nearest neighbor rules of Stone [10] do not have this recursive property. In [11] recursive versions of nearest neighbor rules, which retained the property (1), were given.

The research in nonparametric estimation and discrimination was complemented by Grants AFOSR-77-3385 and AFOSR 76-3062 from the Air Force Office of Scientific Research.

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Research Unit IE8-2 ELECTRONIC MULTI-DIMENSIONAL SIGNAL PROCESSING

Principal Investigator: Professor J.K. Aggarwal (471-1369)

Graduate Students: N.C. Huang and H. Chang

A. PROGRESS: Techniques for processing two- and multi-dimensional signals are under investigation using both recursive and nonrecursive digital filters. The current and proposed research focuses on the synthesis, implementation and stabilization of two- and multi-dimensional recursive digital filters. A program of research has also been undertaken concerning the analysis and synthesis of shift-variant digital filters which have potential applications to seismic data, shift-variant images, radar and sonar signals, and many other areas. Progress has been achieved as follows.

The design of two- and multi-dimensional recursive digital filters with arbitrary frequency characteristics has been difficult due to the absence of the Fundamental Theorem of Algebra in two- and multi-dimensions. Another difficulty with the synthesis of two-dimensional (2D) recursive digital filters is the lack of a stabilization procedure. In view of these difficulties, our research has been directed toward the issues of stabilization, synthesis and implementation of the general class of 2D recursive digital filters. Specifically, we introduce a more general class of PLSI (planar least square inverse) polynomials, termed PLSI polynomials of semicausal form, in an attempt to overcome these difficulties with 2D recursive filters. A new procedure has been developed in [1,3] for the design of semicausal digital filters by utilizing the generalized class of PLSI polynomials. The new procedure requires only a single operation of finding the PLSI polynomials of semicausal form, which is much simpler and more accurate than previous methods.

Recently, the stabilization problem of two-dimensional recursive digital filters has received considerable attention. On the basis of the spectral factorization capability of PLSI polynomials of semicausal form, we present a new stabilization procedure in [2], which offers an effective means for stabilizing 2D unstable digital filters. It does not involve an intermediate PLSI polynomial since stabilization of an unstable filter is directly obtained from its autocorrelation function. The new procedure offers a remedy for flaws in Shanks' original procedure for stabilization. Also, we proposed a new measure of the amplitude distortion due to sta-

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bilization. This measure helps in judging the acceptability of the amplitude response of the resulting filter.

The paper [4] published in the book edited by J.K. Aggarwal reviews recent developments of 2D recursive digital filters in terms of semicausality and factorization, and thus establishes a fundamental theory of recursive filters. The discussions involve stability, stability testing algorithms, the discrete Hilbert transform, spectral factorization, stabilization and design techniques. Specifically, various features of stability have been discussed in the paper for both causal and semicausal filters. In addition, the magnitude and phase relationships for the Fourier transform of a 2D semicausal sequence are derived via the discrete Hilbert transform. Furthermore, a variety of techniques for the design of 2D recursive filters are also reviewed with special emphasis on the design procedure which produces a 2D semicausal filter.

As another approach to overcome the difficulties associated with spectral factorization and stability in 2D recursive filters, we have developed a design technique for approximating nonseparable frequency characteristics by sums and products of separable transfer functions. This approximation is called "piecewise separable" decomposition of the characteristic. In [6,7] the desired filter with half-plane symmetry is obtained by shifting a prototype low-pass characteristic in the frequency domain, and then combining these shifted characteristics with four-quadrant symmetry filters. Although the overall transfer function is a complicated one, the repeated structure within the transfer function reduces this complexity. The advantage of this technique is that the difficulties of stability associated with the nonseparable characteristic do not arise in the present technique. This is a major point in favor of the present method as compared to earlier attempts at the synthesis of nonseparable characteristics.

Nonrecursive 2D digital filters are also widely used in multi-dimensional signal processing, because they bypass the stability problem which is inherent in recursive filters and because they can achieve a strictly linear phase, which is a desirable feature for the distortionless processing of images. However, if the impulse response array has the desired frequency characteristic, the array dimensions may be large and the implementation may be time consuming. In this respect, we have proposed a new technique for the design of 2D nonrecursive digital filters in [8]. To speed up the convolution operation, a high-order impulse response array of a filter may be optimally truncated to give a low-order

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impulse response array. Generally speaking, such optimal filters have impulse responses with non-rectangular arrays (NA). The superior performance of NA filters is apparent from several examples in [8]. Finally, we introduced and demonstrated an efficient convolution algorithm for NA filters.

This report is a brief summary of our accomplishments conducted under the Joint Services Electronics Program in the past year. In addition to the work documented above, three of our previous papers have been republished in the book edited by Mitra and Ekstrom [9-11]. Also, two papers [12,13] will be presented in forthcoming conferences. The first of these two papers [12] provides a starting point and a framework for studying linear shift-variant digital filters which are more effective than linear shift-invariant digital filters in some applications. The present research effort on multi-dimensional signal processing will be continued. We plan to generalize and improve some of the results we have achieved in [1,2,7,12,13] as well as investigate more research problems in this area.

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Research Unit IE8-3. ELECTRONIC CONTROL SYSTEMS

Principal Investigators: Professor R.H. Flake (471-1014)
Professor S.I. Marcus (471-3265)
Professor B.F. Womack (471-3732)

Graduate Students: H.N. Brady and K. Hsu

A. PROGRESS: General theories for the analysis and design of control systems are difficult to obtain and to apply to practical systems. A more promising approach in many cases is to explicitly take into account the system structure, thus deducing more powerful analysis and design techniques which are applicable to a particular class of systems. The final year of this research unit has been oriented toward implementing this approach for control systems consisting of subsystems with a particular interconnection structure, and for systems in which the state is constrained to evolve on a compact surface.

1. Stochastic Systems. An important component in the sub-optimal control of a stochastic system is a state estimator, particularly if the "separation principle" is invoked. A major effort was undertaken to investigate the use of the inherent structure of particular subclasses of nonlinear stochastic systems in order to design high-performance, easily implementable suboptimal estimators for these systems. In particular, the tools of harmonic analysis on Lie groups and homogeneous spaces have been used to design suboptimal estimators for nonlinear systems whose state evolves on a compact Lie group or homogeneous space, such as the n-sphere [1-2]. These models have applications in phase tracking and demodulation, satellite tracking, and rigid body orientation estimation. The performance of estimators designed by these techniques has been evaluated by means of Monte Carlo digital computer simulations, and the results have been favorable. These estimators in many cases performed better than other estimators, such as the phase-lock loop and extended Kalman filter, and with comparable or fewer computations. More specifically, estimation on the sphere is considered in [1]. This problem is motivated by the desire to track a satellite in a spherical orbit about a celestial body, where it is assumed that the orbit is perturbed by random effects which can be modeled by Gaussian white noise. A suboptimal estimator is designed; it performs at least as well, under a variety of parametric conditions, as the extended Kalman filter and the Gustafson-Speyer state-dependent noise filter, and with comparable or fewer computations.

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Similar methods are successfully applied to an optical phase tracking problem in [2]. In this problem, the state of the system is the phase $\theta(t)$, and $\sin \theta(t)$ is used to modulate the intensity of a coherent light source, such as a laser, which is pointed at a remote receiver. As opposed to the previous problem in which the observations consisted of nonlinear functions of the state corrupted by additive white noise, the observation in this problem consists of the output of a photodetector--a doubly stochastic Poisson process with rate modulated by $\sin \theta(t)$. The objective is to estimate $\theta(t)$ given the past observations of the photodetector. Monte Carlo computer simulations have shown that an estimator designed by our technique performs comparably or better, over a wide range of frequencies and noise variances, than the previously used "quasi-optimum" estimator of Snyder for this problem.

2. Interconnected Systems. Several problems in the analysis and design of interconnected systems were addressed. Levins' Loop Analysis method was developed for investigating the behavior of distributed, interconnected systems in which the interactions are not known well enough to be completely modeled quantitatively [3]. The presence or absence and the signs of the interactions between the subsystems may be all that is assumed in the model structure. Previous analysis focused on the qualitative stability, in the small, of the equilibrium points of the system, as well as the possible first order shifts in these equilibrium points due to the influence of constant disturbances. In [3], the loop method was extended to the qualitative analysis of the transient and long term tracking behavior of stable systems experiencing time-dependent and periodic disturbances.

In [4], a study was made of various types of dynamic multiple-connected subsystems which might be placed under direct digital control by a microprocessor. A circular-polar configuration was selected for experimentation. The effects of parameter variations on system stability, system outputs, and performance indices were determined. A control program, suitable for use on a microprocessor, was developed. The program minimized production cost for an experimental system model. A study was made of improvements in control methodology made possible by developing hardware and software technology. This work was extended in [5], where a set of fully interconnected n -th order discrete-time subsystems was considered. The subsystem errors were minimized with respect to the coupling, feedback and forward gain parameters, using nonlinear programming. It was demonstrated that the error functions for subsystems of third order and higher are independent of the

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coupling gains and some of the feedback gains. Increasing the number of subsystems tends to increase the error cost function. These results demonstrate that a judicious choice of coupling, feedback, and forward path parameter gains can substantially reduce the errors in all of the interconnected subsystems.

In further work related to the coupling of subsystems, sensitivity functions were applied to the decoupling problem in [6]. Multiple input/multiple output systems were considered, and classes of decouplable systems were identified. In addition, this research resulted in the development of design methods which utilize sensitivity functions to minimize the coupling to first order in the parameter variations.

All projects in this unit have been successfully concluded. Follow-on projects in the areas of nonlinear estimation and modeling of stochastic systems are being initiated and continued under the Nonlinear Filtering and Estimation Research Unit and National Science Foundation Grant ENG 76-11106.

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Research Unit IE8-4. ELECTRONIC COMPUTER SYSTEM DESIGN AND ANALYSIS

Principal Investigators: Professor S.A. Szygenda (471-7365)
Professor E.W. Thompson (471-1114)
Professor G.J. Lipovski (471-1952)
Professor T.K.M. Agerwala

Graduate Students: M. d'Abreu, E. Pacas-Skewes, B. Rathi,
D. Ross, P. Uppaluru and R. Von Blucher

A. OBJECTIVES AND PROGRESS

1. Design, Simulation and Testing of Digital Systems. The research objectives for this unit included the following: (a) Increase the capabilities of digital logic simulation: both simulation of the fault free network for logic verification and timing analysis, and simulation of the faulty networks for verification of test sets; (b) Increase the capabilities for simulating large networks in a cost effective manner, while maintaining the level of accuracy required; (c) Investigate built-in-test techniques for testing of functional modules.

Significant progress has been made toward achieving the stated objectives. The most significant results include advances in the area of concurrent simulation techniques [1], mappings and algorithms for precise delay gate models [2], and built-in-tests for I/O controllers [3].

The concurrent simulation experimental work [1] centered around the development of techniques for simulating at the functional level, with minimal sacrifice in accuracy. This work concentrated on being able to simulate functional modules, utilizing minimum-maximum delays, and hence propagating ambiguity areas through the network. The algorithms and data structure developed and implemented, support multiple input/output, memory/no memory elements as well as gates. The simulator was designed to handle any number of signal values; the number of signal values comes into play when modeling an element or device.

Since, in concurrent simulation, a fault is handled in the same manner as a good element, accurate timing analysis can be performed to detect spikes caused by the presence of faults. Also, the accuracy of simulating a fault is the same as the accuracy of simulating the non-fault model. The simulator structure supports modeling of any user defined nonclassical faults, such as: (a) functional behavior faults,

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(b) technology dependent shorted signal faults, (c) timing faults, i.e., faults that effect propagation delays and operational timing parameters like setup/hold times, pulse widths, etc. However, in the experimental version of the simulator only stuck-at-faults and timing faults were implemented.

In the simulator, functional elements are modeled independent of the device's internal gate configuration. Therefore, they simulate the device's functional behavior. A J-K flip-flop is an example of a very basic functional element, when modeled by its functional behavior rather than its internal gate circuitry. The flip-flop models have the capability of using different propagational delays, based on the input that is active and operational timing parameters, such as setup/hold times and pulse widths. Checks for violation of the operating timing parameters can be performed for both the good element as well as the faulty element. To accomplish this, the data structure that defines a fault, as well as an element, incorporates the necessary timing information.

The area of mappings and algorithms for precise delay models represents an attempt at establishing some mathematical formalisms in the area of digital logic simulation [2]. Precious little mathematical formalism has been achieved in the past, with respect to parallel fault simulation, modeling, and diagnosis. It is felt that this area has now empirically matured to an extent that permits these formalisms to be developed. It is toward this end that this aspect of the research has been undertaken.

It is obvious that there are different degrees of approximation to the signal values in digital circuits. The more signal states we use in digital simulation, the more information we can expect from the simulated result. On the other hand, the cost to design and implement a digital simulator will increase substantially as the number of states increases. Also, it takes more computer time to complete a simulation run in this case. Consequently one of the major tasks in designing a digital simulator is to select the proper number of signal values. It is usually adequate to use a five-value signal model in design verification and a three-value signal model in fault simulation. A complete analysis of these two models was undertaken. In addition, formal mathematical mappings and algorithms were synthesized for these models.

The built-in-test effort [3] centered around the design of a diagnosable and fault tolerant input/output controller. The approach used is to follow an initial design

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effort by a detailed analysis of the organization of the system and its environment. Based on this analysis, modifications were made on the system and its environment to get the desired performance. For the interface controller under consideration, it is shown that its diagnosability and fault-tolerance can be improved significantly by introducing a minor amount of redundancy into the system. The environment, which in this case is predominantly a CPU or a channel, is modified only to the extent that a nominal amount of software is added and the existing software modified. The overall effect of these modifications resulted in a system which achieves reliability comparable to that of 100 percent duplication, utilizing redundancy of approximately 30 percent.

2. Interconnection Techniques. The use of a Banyan Switch in reconfigurable computers was reported [4] and has led to a grant from NSF to study the architectural properties in general, and a contract from Rome Air Development Center to study applications to communication systems. The proposed work relevant to intelligent discs has resulted in analysis of some unreported aspects of the earlier work done on the CASSM system [5,6]. This work has been directed towards networks of intelligent discs and microprocessors. Due to considerable funding from other agencies, these topics are not being continued under the JSEP contract.

3. Petri Nets and Parallel Systems. The use of live, safe and persistent Petri nets in the design of digital systems has been investigated. Top down and bottom up techniques for the synthesis of Petri nets have been developed. This methodology is equally applicable to hardware and software systems and especially suited to systems exhibiting concurrency. A gate level implementation of transitions allows the direct translation of nets into circuits. The resulting circuits are speed independent. Design verification through simulation requires only 3-valued unit delay simulators, thus significantly reducing simulation problems found in conventional synchronous circuits. Moreover, the circuits have inherent fault detection capabilities. Most stuck-at faults cause all operation to cease. This is an especially useful property for circuits interfacing with weapons systems or expensive peripherals. Other advantages of this methodology accrue from the utilization of a single representation scheme at various levels of abstraction: (a) use of a single simulator for design verification at any stage of the design process, (b) the possibility of performing functional as well as gate level simulation using the same simulator. The above

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work is reported in Refs. 7,8,9.

Significant results have also been obtained in the area of "communication in parallel systems". Models have been developed and communication measures obtained. The importance of communication aspects has been clearly demonstrated and factors affecting the nature and complexity of communication in parallel systems identified. A design methodology which includes both computation and communication aspects has been developed. Except for the initial stages [10], this work has been supported primarily by a grant from the National Science Foundation. The work on Petri nets and parallel systems under JSEP funding has been terminated since Professor Agerwala is now employed by the IBM Thomas J. Watson Research Laboratory.

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Research Unit IE8-5. ELECTRONIC COMPUTER SOFTWARE SYSTEMS

Principal Investigators: Professor R.T. Yeh (471-4353)

Graduate Student: S. Koch

A. PROGRESS: We are continuing our efforts in research into design methods for data base systems and software in general. We have come to the conclusion that the disciplines of software engineering and data base management can benefit greatly from each other. In fact, we believe that a unified design methodology can be achieved.

1. Towards a Unified Design Methodology for Software and Data Base Systems. We discuss a development methodology which will emphasize the separation of concerns for modeling, design, and implementation as well as evaluation at all phases of development. We believe that systems resulting from applying the proposed methodology will be more reliable, because the design is constantly being monitored and easier to modify. This is due to the separation of concerns, which allows the system structure to faithfully reflect the problem structure so that a small change in the environment will only affect a correspondingly small change in the system.

a) Modeling. It was pointed out in [Yeh, et al, 1978] that the process of engineering requirements involves three main activities: problem recognition and description, problem understanding, and solution space specification.

To achieve understanding in the absence of a system, analysis on formal models becomes necessary. It should be noted that mental models about the problem always exist in the minds of the users, analysts and designers. However, for complex systems, such implicit models are inadequate because of the inherent complexity of the system as well as the fact that mental models tend to be incomplete and ambiguous. It is therefore necessary to construct an explicit model from the beginning and use it as a basis to facilitate a process of integration, consolidation and refinement of different internal models or views, as well as for analysis, to aid a designer's understanding of the problem.

The modeling stage is a process triggered by the recognition of certain needs. The analysts then analyze these needs and map them into a conceptual model. In doing so, they are supported by existing theoretical knowledge (e.g.,

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system theory, knowledge about the problem domain, etc.), and their own experience.

The modeling process is thus that collection of activities (e.g., information gathering, problem elaboration and decomposition, etc.) which develops the model starting with a given set of "needs statements." Since conceptual modeling is primarily used for problem understanding, we may regard a model as a complex "knowledge structure" which consists of a highly structured collection of concepts and their interrelationships. As a consequence, an analyst, for example, can gain understanding of the problem by "navigating" through this knowledge structure. It should be noted that in order to "design for change," the conceptual model not only needs to model a system, but also the environment in which the system is embedded.

The conceptual model, being a result of consolidating many different views, may contain a great amount of redundant information. While redundancy facilitates understanding, it may not be desirable for specification. For example, the model may contain information concerning possible ways of implementing a system which may constrain a designer's freedom. We view then the specification as that minimal set of essential information extracted from the conceptual model which can completely characterize the system to be developed. We may view it as a set of "valid projections" of the conceptual model in the same way that an architect represents a proposed 3-dimensional building in terms of 2-dimensional views - top view, side view, cross sections, etc.

But what needs to be modeled? Although it is correct and precise to characterize a software system as a "large computer program" and to be concerned with problems of efficiency, performance, resource allocation, etc., software systems can also be considered from another point of view, namely, as "models of reality." If, for instance, we consider an information system for a hospital, or a real-time system that controls chemical processes, or an operating system that allocates and manages computer resources, we see that those systems, to a large extent, reflect the environment that they have to control and the policies or goals of the organization to which they belong. In this sense we say that software systems are "models of reality." Furthermore, these systems do not exist in isolation but they are "embedded" in organizations.

A software system is part of a more global man-machine system, which we will call an Information Processing System (IPS). The IPS is, in turn, one of the components of an organization which is governed by a set of goals. These

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goals (which can constitute a rather complex structure, ranging from very abstract goals to highly specific policies) provide a context for the interaction between different components of the organization and for the interaction between the organization and the external environment. The complexity of these relations makes apparent the diversity of forces that operate upon a software system forcing it to enter in a process of evolution to maintain its adaptation.

From this perspective it appears to be important to reach a high level of understanding of the environment and the set of goals or policies that constitute the context of the software system, and this is precisely the rationale for the development of explicit conceptual models. Once the idea of conceptual modeling has been accepted, the following questions arise:

- Which are the aspects of the "environment" that are relevant to a system?
- What kinds of changes in the "environment" may affect the structure of the software system?
- How does the structure of goals and policies of an organization affect a software system?

Notice that the questions have been asked in a general sense, aiming at those kinds of phenomena that are relevant for every software system. We illustrate this by analyzing one aspect of the environment which has a deep effect on the structure of a system.

The environment of any software system can be partially characterized as being constituted by a set of entity classes, each one with a well defined set of attributes. Instances of these classes are characterized by specific values of the corresponding attributes. The attributes of entity classes are interrelated by different kinds of relationships. For example, an attribute of an entity class may be such that given a value for it a specific instance or set of instances of another entity class may be uniquely identified.

Different systems and their environments have distinct characteristics. In order to be able to describe system and environment pairs, it is important to extract from a class of systems certain common characteristics which can be utilized for descriptive purposes. These characteristics may be axiomatized. We propose here the basic structure of a model for information system. This model can be considered as a collection of units of several types. The units are partitioned into three sections: environment, interface, and

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information system. Such a characterization can provide a scientific basis for analyzing the problem space so that an analyst can quickly focus on different aspects (both static and dynamic) of the system, and that "design for change" can be facilitated. (Note that data base design as practiced now only models the information system and not its environment.)

To summarize, we have expressed previously that conceptual modeling is concerned with two major tasks: problem understanding and solution space specification. Thus, research investigations should be dealing with the construction of complex "knowledge structures" to aid our understanding of the problem, and develop perhaps a "simpler" model to delineate the solution boundary. We must, of course, also look into the transformation from one model to another. An example of this two model approach in (static) data base design is given in [Yeh, Chang and Mohan, 1978].

We believe that the model for understanding basically consists of a highly structured collection of concepts and their interrelationships that have three distinct aspects.

- (1) A description (model) of a proposed system and its environment (perhaps at several levels of abstraction);
- (2) A description of the decision process that led to the construction of this model;
- (3) Built-in knowledge that corresponds to the concepts that constitute the knowledge structure.

The model that is used for specification should differ from the understanding model in that it should contain only essential information, i.e., minimal redundancy should exist.

b) Design. Although much attention has been paid to the design issues in the last few years, many of the design techniques are still inadequate for the following reasons.

- (1) Design is not evaluated at all stages.
- (2) There is no provision for documenting the design process, e.g., why a particular decision is made among many alternatives. Such a documentation is important for developing evolutionary or portable systems.
- (3) There is no provision for documenting the system structure. Although it is generally agreed that the system is hierarchical in structure, many hierarchies may coexist, each representing a different relationship between system components.

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To alleviate some of the design problems just mentioned, an enhanced methodology was proposed in [Yeh and Baker, 1977; Chester and Yeh, 1977]. In current practice the design model can be considered as both a model of the design structure, and (primarily) as a model of the system structure. In order to allow explicit documentation of the design process, the enhanced methodology proposed the separation of design structure and system structure as well as adding an evaluation model such that all three models are refined together during software development. The reader is referred to the two papers cited above for a more detailed description of this methodology.

The design phase then begins with a conceptual model and ends with a system architecture (SA). The SA is intended for two purposes: (1) to serve as a blueprint for system implementation. In this sense, it is a "completely documented abstract machine"; (2) to serve as a mock-up model for users' final check before implementation begins.

c) Implementation. Major advances in software methodology have been made in implementation techniques during the last decade and we shall not elaborate on this aspect here.

2. A Data Base System Design Methodology. In this section we shall briefly describe a design methodology for data base systems as an example of the methodology proposed in the previous section.

A Data Base System (DBS) is a software system utilizing some data base management system (DBMS) functions as its building blocks. Information systems that do not utilize DBMS's usually also require management of some data structures. A DBS design methodology should therefore be easily extendable to a methodology for designing general information systems.

The design of a DBS includes two parts: the design of the data base and the design of the programs utilizing the data base. As is done today, both parts of the design are artistic in nature and must depend on the individual experience of designers. Such design practices often produce inefficient, inflexible and inconsistent DBS's which can potentially be disastrous to the enterprise employing them.

The design of data bases has been addressed by the researchers in the data base field. Earlier efforts were mostly concentrated on the design of physical storage structures in data bases. Recently, much work was done in the logical design area. However, no comprehensive methodology has been developed. Most of the research was aiming at

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solving a small portion of the design problem with some restrictive assumptions.

The design of programs in a DBS has not received much attention. With the recent advances in the software engineering area, however, we believe that it is possible to include in a DBS design methodology the techniques for DBS program design.

Yeh [1978a; 1978b] described our multi-level approach to the DB design problem. The first step in the design is to obtain a conceptual schema of the information structure; then the conceptual schema is mapped into a logical schema. The details of physical storage structures are designed in four more levels of mapping with each level introducing more implementation decisions.

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II. SOLID STATE ELECTRONICS

SOLID STATE ELECTRONICS

Research Unit SS8-1. BASIC SOLID STATE MATERIALS RESEARCH

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A. OBJECTIVES AND PROGRESS

1. Solid State Reactions at Metal-Semiconductor Interfaces. One of our objectives is to develop a physical model for the kinetically selected reaction paths and the thin film phases in solid state reactions observed at metal-semiconductor interphases. Another objective is to correlate the time development and properties of these reaction paths with the electronic and mechanical properties of the resultant interphase structures.

Previously, we made some progress in understanding part of the structure and basic mechanisms involved in the interfacial reaction. This led us to postulate the formation of a membrane phase [1,2] which determines the formation of the first crystalline phase nucleated under normal experimental conditions. We have shown how the interphase structure postulated is consistent with Schottky barrier properties [3], particularly in terms of the pairing of states near the Fermi level in the interfacial region. Finally we have observed the structural formation of ultrathin films of Ni and Co sputtered on Si single crystal substrates in a technical vacuum. We have found the formation as a function of thickness, consistent with our hypothesis of the formation of a glassy state prior to first compound formation.

In our experiments on ultrathin nickel films rf sputtered onto both (100) and (111) silicon, we have found amorphous surface regions (via Transmission Electron Diffraction (TED)) in the equivalent thickness range $10 \leq t \leq 28\text{\AA}$. Auger electron spectroscopy (AES) measurements indicate no contaminants in these thin layers. Annealing 10\AA films at 400°C for one hour does not alter the TED pattern. At 15\AA , however, the anneal produces polycrystalline rings of $\delta - \text{Ni}_2\text{Si}$. In unannealed samples, Ni_2Si polycrystalline rings are seen at a minimum deposited metal thickness of 30\AA and AES measurements show a splitting of the 92eV silicon line previously reported for Ni_2Si . Both NiSi and Ni_2Si polycrystals are seen via TED at a deposited thickness of 120\AA upon anneal at 300°C for 30 minutes. These measurements also indicate that Ni_2Si is nucleated from an amorphous

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region whose structure (as indicated by TED) is independent of the amount of Ni sputtered onto the substrate.

Our experiments on ultrathin films of Co deposited on Si single crystal substrates have shown essentially the same results. The thickness for Co_2Si nucleation upon deposition at room temperature appears to be a little thicker-- approximately 40 \AA . This nucleation thickness is a sensitive function of substrate preparation and cleanliness. The thickness increased (at low rf sputtering voltages) if the surface layer of oxygen on the Si was not backspattered off prior to the deposition.

For the Co-Si system we have recently correlated the thickness for which Co_2Si nucleates out of the glassy layer with the resistance properties of the layer. What we have found is that the onset of first phase nucleation begins at the semiconductor-metal transition in the glassy layer.

(Determined by the thickness where $\frac{dR}{dT} \rightarrow 0$.) The surface resistance where this takes place is in the range of $10^3 \rightarrow 10^4 \Omega/\square$, thus indicating that crystallization occurs when the glassy layer obtains a region of two-dimensional metallicity [5]. We are working on possible models which we have proposed involving cooperative, long range coupling over the interface of local atomic modes via the delocalizing electronic system. The coupling may be either via single electrons or to a cooperative electronic system such as a "Wigner liquid."

We are presently following up this correlation with measurements on other systems (Ni-Si, Fe-Si, Pd-Si), and are also making noise measurements and magnetic measurements (EPR) in order to determine more fully the properties of intermediate structures along the reaction path, and the approach to criticality of these parameters as we approach a phase transition. In addition, optical experiments have been begun as described below.

2. Optical Experiments for Surface Studies. Our objective in this work is to determine the range of experimental parameters which yield the optimum information from ellipsometer studies of interfaces. We have previously developed interactive graphics software for use in the ellipsometric determination of optical constants of a thin film (known thickness, known substrate), and have tested it on both real and "artificial" data. This work has allowed us to determine a priori the regions of N-K space and incident angles which should be studied experimentally to get the best physical information.

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The optical interface characterization study has progressed from numerical simulations to experimentation on the problem of immediate interest, namely the Co-Si interface region. A combination of numerical simulation and preliminary experiments has indicated that a satisfactory set of data can be obtained by first obtaining curves of ψ and Δ versus angle of incidence at about ten evenly spaced angles, and then obtaining many more data points in regions where structure (peaks, dips, etc.) is seen in the preliminary curves. The reduction of experimental data is accomplished by a least-squares curve-fitting program. Thus, the use of many data points in regions where ψ and Δ vs angle of incidence shows structure weights the curve-fit towards those regions. Even for very small ($<50\text{\AA}$) deposits of Co, the experimental differences between the Si substrate with only a thermal oxide layer on the surface, and the same substrate with Co deposited, are quite pronounced. For example, the pseudo-Brewster angle, when ψ passes through a minimum and Δ changes very rapidly with angle of incidence, increases sharply with the deposition of Co. For substrates with very thin surface films, it is often claimed that the pseudo-Brewster angle gives a measure of the substrate refractive index. In our experiments, this is true only for the Si with just the oxide layer on the surface, when the pseudo-Brewster angle was found to correspond to a substrate refractive index of 3.88 at the 6328\AA measuring wavelength in good agreement with other bulk Si data in the literature. With even a very thin Co deposit, the substrate index one would infer from this measurement increases to 4.80, which is obviously uncharacteristic of the bulk Si substrate.

We plan to interpret, using the curve-fitting procedure described above, these results in terms of two interface models: first, a single composite layer on a bulk Si substrate; and second, a SiO_2 layer on a modified surface layer on bulk Si. The optical properties of this surface layer will be obtained for different substrate doping conditions and Co deposit thicknesses, and correlated with TEM and TED experiments on similar samples described elsewhere in this report.

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Research Unit SS8-2. RESEARCH ON INSTABILITIES AND TRANSPORT NEAR SURFACES AND INTERFACES OF SOLIDS

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D. Sheng

A. PROGRESS: The broad objective of the research described in this unit is to gain an increased understanding of the relationship between atomic rearrangements and electronic instabilities at surfaces and interfaces of solids. Our previous studies of compound nucleation and recrystallization have led to the speculation that the thermal reaction path of interfacial chemistry in solids may be determined by the fluctuations of redistributed, or delocalized, bond charge.

At this time our work is aimed at 1) developing experimental techniques for producing and characterizing several model interfacial systems, 2) studying the thermally and non-thermally driven reaction kinetics of these model systems, and 3) developing theoretical models for the interfacial chemical kinetics. The following describes the specific objectives of our current research tasks and the progress made thus far.

To investigate the effects of electric fields, we are using the Pt/Si planar reaction couple. We are specifically interested in investigating the influence of electric fields on the kinetic course of the subeutectic silicide-forming reaction in this particular model system. Work on this research has been divided into both theoretical and experimental investigations. The theoretical investigation has initiated the development of the understanding of the influence of applied fields upon second phase stability and growth processes [1-5]. The research involved a set of simultaneous continuity equations which may be solved to simulate the morphological evolution of a second phase. Recent emphasis has been on the understanding of flux discontinuities that arise at phase boundaries and at sample end conditions [1,5]. Such flux discontinuities provide positions where the solute correlation may significantly depart from equilibrium and lead to a diffusion kinetic basis for precipitate growth (in contrast to a thermodynamic one). Hence, it is found that solute solubility near a phase boundary depends upon several factors, including a) distribution of the second phase to act as a solute sink/source, b) field

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strength that is capable of rearranging the solute composition, and c) magnitude of the flux discontinuity. Although progress to date has emphasized simple morphologies that can be modeled analytically, the above characterizations are general and should apply independent of morphology. As a consequence, the understanding of a simple planar interface as found in the metallization of silicon has been implemented by these investigations.

Experimental work has been confined to the planar Pt/Si system. The long-range emphasis is to understand the role of external electric fields upon the reaction at sub-eutectic temperatures. The Pt/Si system was chosen to provide a transition metal that reacts well with silicon but is not influenced by problems of oxidation. The initial experiments were designed to determine the extent to which platinum reacts with silicon at room temperature. With very thin layers of platinum, in the range of 10 to 75 \AA , we find with TEM that the layer of platinum is amorphous upon deposition in thicknesses of up to 30 \AA . The glassy film is characterized as a semiconductor through measurements of sheet resistance as a function of temperature. A transition to a metallic compound is found at thicker layers of deposited platinum (about 40 \AA). The compound is identified as Pt_2Si . We have had extensive concern about the role of oxygen contamination during preparation and have, therefore, standardized the sample preparation procedure. Current experiments indicate an increased stability of the glassy film as a consequence of a decrease in oxygen during sample preparation. We are confirming this using Auger electron spectroscopy. Initial experiments on the effect of an applied electric field during platinum deposition are inconclusive and reflect sample preparation that did not conform to our current standard practice. In fact, the inconclusive nature of these experiments provided the motivation for standardizing the sample preparation. We are, therefore, in the process of repeating the early experiments on electron injection during platinum sputtering using the standardized sample preparation. The work is continuing.

The study of the effect of electric fields on interfacial chemical kinetics is expected to enhance our understanding of solid state electromigration and is one of our two basic studies of non-thermally excited interfacial reactions. In the other we are investigating the role of optical excitation. At present we are trying to understand optical selection rules for driving the well characterized 68°C martensitic structural transformation in VO_2 thin films. We expect that this type of cooperative, long-range, diffusionless transition may be important at interfaces, too.

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However, in spite of their enormous technological importance (e.g., in steelmaking) their physics is not yet well understood.

Previously we had reported on our observation that a unique non-equilibrium state could be induced in VO_2 by 41 psec and 22 nsec pulses of 1.18 eV photons at 341°K. We have subsequently found that this state decays by a complex two-time constant process with the overall decay time increasing from one μsec to over one msec with increasing ambient temperature and pulse energy [6,7]. It is important to note that the thermal equilibrium state could not be accessed by short ($\lesssim 20$ nsec) 1.18 eV photon pulses of any magnitude. Recently we have speculated that this result indirectly confirms recent models which view this transformation as a Fermi surface-related soft phonon mode anomaly driven by charge density excitations. In our experiments, we believe this instability is preempted by fast population of alternative electronic states not related to the crystalline structure, i.e., localized states.

More recently [8,9] we have observed evidence of coherent excitation phenomena in the excited transmission state response of the VO_2 films to ~ 33 psec pulses from the Nd:YAG laser. The initial transmissivity is observed to increase for a time shorter than that of the pulse ultimately decaying to the non-equilibrium state observed in the other experiments. This suggests that fast relaxing coherently prepared electronically excited states may be present, but these are not necessarily directly involved in the structural rearrangements, which are observed for considerably longer (~ 20 nsec) pulses.

We have also completed a study of the interface resistance of VO_2 films of various thicknesses prepared by CVD on single crystal quartz and sapphire substrates, to further investigate the role of the transition layer on their electronic stability [10,11]. We have not completed the analysis of this data as yet; however, the results support our previous work showing that a transition region of anomalous resistivity exists at the sapphire interface and controls the electro-thermal stability of these films. It is quite remarkable that films thinner than 100\AA on sapphire have undetectable resistance until the phase transition, where one sees the expected jump in conductivity. This line of research is expected to have profound implications for the electronic stability of electronic barriers, contacts and surface films.

Finally, we have recently designed and constructed a low temperature tunneling spectrometer with which we will

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search for molecular-like interface electronic states that may be important to interface chemistry. We expect these to be within a few tenths eV of the Fermi level and to be accessed by inelastic transitions of tunneling electrons. We have recently evaluated the sensitivity of this spectrometer to changes in the intensity of second derivative lines. This is expected to be important in the detection of cooperative interface transitions.

All of the research described above is in a partial stage of completion and will be continued in the next JSEP contractual period. There will be an increased perspective to this research with a major emphasis on the investigation of nonlinear spectroscopic techniques for probing and exciting structure-determining states at transitions. New research on computer simulation of stochastic reaction kinetic processes at interfaces will be initiated by Prof. J. L. Turner.

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III. QUANTUM ELECTRONICS

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Research Unit QE8-1 NONLINEAR WAVE PHENOMENA

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mann

A. Progress: This unit is concerned with analytical and experimental studies of nonlinear wave phenomena in physical systems. The work is subdivided into the following two areas: (1) development of digital time series analysis techniques suitable for analyzing and interpreting fluctuation data generated by *nonlinear wave interactions* in various media, and (2) *nonlinear optics* in the infrared.

Nonlinear Wave Interactions: The objective of this work is to develop digital time series analysis techniques that may be used to analyze and interpret experimental fluctuation data associated with nonlinear wave phenomena. During the past year, our research has focused on utilizing higher order spectral concepts to accurately and completely characterize the "nonlinear" fluctuating signal. Nonlinearities result in new spectral components being formed which are phase coherent; furthermore, the detection of such phase coherence may be carried out with the aid of higher order spectra. In particular, we have concentrated on the bispectrum, a function of two-frequency variables, which is suitable for analyzing quadratic nonlinearities. (Higher order nonlinearities will require higher dimensional spectra.) Utilizing the results of regression analysis and least mean square theory, we are able to define a bicoherence spectrum [1] which basically measures the degree of phase coherence between three waves due to (quadratic) wave coupling. We demonstrated in Ref. [2] the usefulness of the bicoherence spectrum to discriminate between nonlinearly coupled waves and spontaneously excited independent waves in a self-excited fluctuation spectrum. In addition, it was shown in Refs. [1,3] that the squared value of the bicoherence spectrum measures the fraction of wave power present in a spectral band centered at frequency ω which is due to wave-wave interactions of a quadratic nature.

We have also investigated important practical aspects of digital bispectral analysis, and in Ref. [1] report

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that the estimators are statistically stable when the interacting waves are quadratically coherent and relatively unstable when the waves are quadratically incoherent. In such incoherent cases, the variability of the estimator can usually be reduced by ensemble averaging over an increased number of realizations. Furthermore, the effects of noise on the bi-coherence spectrum estimates have been examined. We found that the value of bicoherence is reduced by a factor of $[(1 + \alpha(\omega_1)(1 + \alpha(\omega_2))(1 + \alpha(\omega_1 + \omega_2))]^{-1}$ where $\alpha(\omega)$ is the reciprocal of the signal-to-noise ratio.

We have placed a great deal of effort in understanding the relationship between the measured bispectral quantities and the physics of nonlinear wave interactions. As waves propagate through a nonlinear dispersive medium, a temporal and/or spatial variation (i.e., modulation) in the wave's (complex) amplitude may result from competition between the dispersiveness and the nonlinearity of the medium. Let $\Phi(\omega)$ be a Fourier amplitude measured at a spatial point. Then, $\Phi(\omega)$ will satisfy

$$\frac{\partial \Phi(\omega)}{\partial x} - ik(\omega)\Phi(\omega) = \sum_{\omega_1 + \omega_2 = \omega} V_{12}\Phi(\omega_1)\Phi(\omega_2) \quad (1)$$

where $k(\omega)$ is a function of ω and describes the dispersiveness of the medium, and V_{12} is the coupling coefficient for the nonlinear interaction of waves present at ω_1 and ω_2 . From Eq. (1), we made the following interesting observations for three-wave coupling [4]. For example, the biphase, the phase of the bispectrum, is determined by the characteristic scale length of amplitude variation due to nonlinear coupling and the phase of the coupling coefficient. Furthermore, when the coupling coefficient is real and positive, the sign of the skewness⁺, which is determined by the biphase, can be explained in terms of nonlinear wave characteristics. That is, if the wave's amplitude is growing in the direction of propagation, a negative skewness results and if the amplitude is decaying, a positive skewness results.

In addition, we have considered the power variation of a wave in terms of the bispectral power transfer function, which involves the coupling coefficient and the bispectrum. When the coupling coefficient is known a priori, one can experimentally determine the direction and the amount of

⁺Skewness is defined as the mean cube value of a fluctuating signal divided by the cube of its standard deviation.

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power transfer over a spectrum due to nonlinear wave coupling by utilizing bispectral techniques.

In many experimental situations, it is often desirable to model the relationship between two (or more) physical quantities. We have concentrated on developing techniques and procedures whereby this modelling may be carried out in terms of both linear and quadratically nonlinear systems. The approach is to model the relationship either in terms of linear and quadratic impulse responses in the time domain, or linear and quadratic transfer functions in the frequency domain. For a noncausal case, the frequency domain modelling is relatively straightforward. Using the results of least squares theory and multiple regression analysis, we showed in Ref [5] the best (in a least mean square error sense) linear and quadratic transfer functions may be expressed in terms of a cross-power spectrum and a cross-bispectrum (respectively) between input and output. We also demonstrated that the cross bicoherence spectrum represents the fraction of power present in the output at frequency ω (or mean square value) which can be accounted for by the quadratic nature of the system [5]. Contrary to the noncausal case, modelling a causal system in the frequency domain is not straightforward, since causality requires the impulse response to vanish for the time interval before the impulse was switched on. Modelling a quadratic causal system by a Volterra series truncated after the second-order term and utilizing an approach similar to that associated with a linear Wiener filter, we obtained the optimum quadratic impulse response and quadratic transfer function [6].

From a basic scientific and research viewpoint, the development of appropriate digital time series analysis techniques suitable for analyzing and interpreting fluctuation data associated with nonlinear wave phenomena is very important in its own right, since such techniques offer *experimental* insight into various aspects of nonlinear phenomena which, in many cases, simply is not available using conventional approaches. At the same time, however, we believe these same techniques, or variations of them, have a very high potential to impact favorably in a number of important technological and/or scientific areas, for example, signature analysis of both electromagnetic and acoustic radiation, certain nonlinear diffraction problems, and nonlinear structural transfer functions in certain important classes of aerodynamic problems. It should be stressed that these are merely examples of potential applications and we, by no means, mean to imply that the potential applications are limited to these areas. In fact, we are convinced these same techniques can be fruitfully utilized whenever the basic underlying physical

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phenomena can be modeled in terms of nonlinear wave or mode interactions.

Nonlinear Optics: The objectives of the work in nonlinear optics have been to study new types of molecular nonlinearities in the infrared. We develop and test theories for the new nonlinearities and demonstrate, test, and optimize devices based on the newly developed theories.

Over the previous reporting period, we have continued the study of high energy, resonant excitation in SF₆ [7,8]. The saturation of the linear and nonlinear properties of SF₆ has now been observed under various conditions. In our laboratory, we have made saturated absorption and third harmonic generation measurements on pure SF₆ at low pressures where collisional effects may be ignored.

The nonlinear susceptibility of SF₆ is strongly affected by multiphoton resonances and by population redistribution and depletion. The third harmonic generation spectrum for SF₆ was measured for intensities above and below the molecular dissociation threshold. Experimental evidence indicates the presence of several resonant multiphoton transitions in the discrete states below 3000 cm⁻¹ and one or two photon transitions from the discrete states to the quasi-continuum, depending on the frequency of laser excitation. In this way we are able to probe the excitation of the SF₆ molecules through the discrete states.

Preliminary third harmonic generation data has been taken on a new system, NH₃ gas. In NH₃ the triple resonance is only approximate. One photon absorption is avoided by tuning the excitation laser between discrete absorption lines. A two photon resonance is selected and is nearly exact, while the three photon resonance is detuned by as much as 10cm⁻¹. The experiments show moderately low third harmonic conversion, as predicted by theory due to the small population on the resonant rotational energy level at room temperature.

We have successfully completed [9] a study of third harmonic generation in gas filled metal-dielectric wave-guides with CO as a nonlinear media. The third harmonic conversion was enhanced in the waveguide because the focused area is independent of the interaction length. For unconfined, focused laser beams these two parameters are inversely proportional and their effects cancel in the overall conversion efficiency. In our work, the theory for third harmonic generation in waveguides was developed. The conversion efficiency was calculated, based on this theory, and measured experimentally. The comparison was good considering the somewhat rough quality of the optical waveguides and of the custom cylindrical focus-

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ing optics used. Measurements were also made using unconfined, focused laser beams in order to demonstrate the enhancement provided by the waveguide configuration.

Study of SF₆ and NH₃ will continue in the coming year. Cryogenic experiments have been initiated in order to simplify and concentrate the vibrational-rotational spectra of these molecules. Much of this work, however, will be continued under the support of AFOSR-78-3712 "New Nonlinear Optical Process in Molecules at Infrared Frequencies," September 30, 1978 to September 39, 1980.

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Research Unit QE8-2. ATOMIC AND MOLECULAR ELECTRONIC PROCESSES

Principal Investigators: Professor L. Frommhold (471-5100)
Professor M. Fink (471-5747)

Graduate Students: W.S. Burns, M.H. Kelley

A. RESEARCH OBJECTIVES: Whereas the scattering of light by non-interacting atoms or molecules is well understood, scattering and attenuation of light by gases at atmospheric or higher density is less thoroughly known [1]. Under such conditions transient quasi-molecular complexes occur, both collisional complexes of free atoms and bound van-der-Waals clusters, which feature a tensorial, incremental polarizability [2,3]. This diatom polarizability is in excess of the sum of the atomic polarizabilities and generates the virial contributions to the light scattering properties of real gases. Binary collisional complexes and van-der-Waals dimers, the so-called "diatoms", scatter light with an intensity that is proportional to the square of the gas density [4]. At extremely high pressures, one will also find contributions from complexes consisting of three, four, etc. atoms (which may be bound or free), each with an identifiable intensity proportional to the third, fourth, etc., power of density [5].

This research concerns the diatoms of the rare gases, and of simple other gases (like hydrogen and the atmospheric gases). It attempts to record their two Raman spectra: the polarized one, which is generated by the trace, the spherically symmetric part of the diatom polarizability tensor; and the depolarized component due to the anisotropy. Each spectrum consists of a continuum (i.e., the collision-induced part) and a weak low-frequency rotational dimer band. All spectra are obtained with a calibration of the absolute intensity. In this way, diatomic light scattering cross sections are determined as functions of the frequency shift. Hand in hand with this spectroscopic work, wave-mechanical computations of the diatom spectra are undertaken, for a direct comparison with the experiment. Models of the diatom trace and anisotropy (which have been calculated ab initio

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for the case of helium [6], but must be somehow constructed for the molecular and heavier rare gases) are used as input. It is easy to judge by the quality of the fit, the accuracy of the employed model, which can then be modified and refined until the resulting theoretical spectra agree with the experiment. This is an important goal of the work. Such work makes use of the collision-induced spectra of the free diatoms. The dimer spectra, on the other hand, are to be used for the first direct measurement of the dimer concentration in a situation of thermal equilibrium. Furthermore, the vibrational and rotational energy levels of the dimers can be obtained from the Raman spectra. With such information, the currently best available semi-empirical interatomic potentials [7] can be given their ultimate refinement.

We mention that the invariants of the diatom polarizability can be measured by only one alternative method. The trace can be determined from a virial expansion of the dielectric Clausius-Mosotti function, and (at the frequencies of light) of the analogous refractive index [8]. The anisotropy is related to the second virial Kerr coefficient [9]. For any given temperature, both methods result in a simple number, usually with a substantial error. Measurements of these quantities, where they exist, were made at only one temperature, severely limiting the information available from such measurements. In contrast, our spectroscopic method yields a spectral distribution function on an absolute scale. The shape of this function carries much retrievable additional information, and measurements at a fixed temperature are usually sufficient for a complete definition of the diatom polarizability model. With regard to the refinements of the interatomic potentials, we mention that essentially all alternative measurements have already been pushed to their limits [7]. Thus, there exist, even among the most highly refined potential functions, minor differences (especially of their shapes) that cannot at present be resolved [7]. Energy levels are known for some van-der-Waals dimers [10], but more work to supplement and verify the existing data is needed. If complete energy tables are obtained, the model potentials can be adjusted to be consistent with this new information. In this way the inherently high precision of spectroscopy can be utilized for the purpose.

Low energy elastic electron scattering in the energy range of 10 eV-1000 eV is a research tool used to study the dynamic response of an atom or molecule to an incoming electron. If the electron is very slow, then the induced distortion in the charge density is adiabatic [11]. The consequence for the cross sections is a strong enhancement at small

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angles, due to the long range dipole field, which the targets produce to shield themselves from the perturbing field generated by the incoming electron. When the electron energy is increased the overall angle cross section decreases, indicating a dynamic response of the molecule [12]. At very high incident energy the electron cloud is too slow to adjust to the incoming perturbation, and the cross section reflects the static potential. It is the latter process we have utilized heavily and were able to exploit to such an extent that we could determine the static distribution of the electrons involved in the molecular bond forming process [13]. (This research is now supported by NSF.) It is now our intent to extend our research to the medium and low energy range.

Electrons which interact with atoms and molecules in the 10 eV-1000 eV energy range have a high probability of exchanging energy with the target. This process has its analog in the optical domain in the Raman spectra. The lines in the inelastic electron scattering spectrum correspond to Stokes lines, while those in the super-elastic spectrum correspond to anti-Stokes lines. There are two important distinctions between the two methods: the cross sections are 8 to 10 orders of magnitude different to the advantage of electron scattering; and spin flip reactions are impossible to study by optical spectroscopy. While the cross sections difference can be decreased by a couple of magnitudes by resorting to resonant Raman scattering, the second argument remains true.

The following analogies can be established:

absorption spectroscopy $\hat{=}$ inelastic electron scattering

emission spectroscopy $\hat{=}$ superelastic electron scattering

Developing the field of superelastic electron scattering is equivalent to a new field of spectroscopy in which the high resolving power of optical spectroscopy is utilized in the excitation of a specific molecular state by resonance absorption. At the same time the de-excitation via electron scattering opens the opportunity to study singlet-triplet conversions, vibrational mode coupling and potential curve crossings due to the selection rules as they apply to scattering processes. This technology has been successfully tested on Na and Ba vapors and therefore looks very promising for the extension to molecular gases [14,15].

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B. PROGRESS: The field of collision-induced light scattering came into existence eleven years ago, by the pioneering work of Birnbaum and McTague [4]. With the review article one of the principal investigators is presently compiling, the major bulk of such work is currently brought to a successful conclusion [16].

More specifically, we mention that collision-induced spectroscopy was relatively easy to do in the highly polarizable gases (Ar, Kr, Xe, CH₄, etc.). By properly optimizing the apparatus, it is possible to obtain in such gases signals amounting to hundreds of counts per second, at gas densities low enough to suppress all three-body contributions. Apart from determining the light scattering cross sections of pairs of atoms, one derives from such measurement models of the anisotropy of the diatom polarizability. Unfortunately, since precise Hartree-Fock type computations of the diatoms are presently not possible for these gases, these models cannot be compared with ab initio calculations of the diatom polarizability. Ab initio polarizability data [6] exists only for helium at present. It was often thought, however, that the experiment in helium is impossible [17]. Indeed, the signals are expected to be four orders of magnitude less intense than, for example, in argon. However, by developing and perfecting a computer-controlled Raman apparatus, for that specific purpose, we were able to record helium spectra [18-20]. Absolute cross sections for scattering of light by collisional pairs of helium atoms were obtained. By comparing the two Raman spectra, one with the polarization of the incident beam perpendicular to the direction of the observation, the other parallel, we were able to show that in helium we have both a polarized and a depolarized spectrum. This constitutes the first observation of a polarized collision-induced Raman spectrum in any gas [19,20], and a new (the second) measurement of the trace. (The first measurement of the helium diatom trace was based on the virial expansion of the dielectric function [8]; it is consistent with the present new measurement.) At the same time, the first measurement of the helium anisotropy is obtained [18,20]. The comparison of these polarizability invariants with their ab initio calculations is generally satisfactory after certain frequency ("dynamic") corrections have been made. Already our work has stimulated new and more sophisticated ab initio calculations of the dynamic diatom polarizability (the first such calculations for helium).

The neon diatom features a collision-induced spectrum which is also extremely weak. Only one other measurement of the neon depolarized spectrum existed [12]. With

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the computer-controlled system developed for helium, it is not too difficult to also record the neon Raman spectra [21]. We were able to verify, and to extend to higher frequencies, the earlier measurement of the depolarized spectrum, and to obtain for the first time the polarized neon spectrum. At the same time, the light scattering cross section of neon diatoms is determined. Empirical accurate models of trace and anisotropy were obtained and compared with theoretical models, which were shown to be inadequate [21]. (This is not too surprising, since the neon diatom is a 20 electron system and too big for accurate computational work.)

Since previous work in argon [22,23], krypton [24], and xenon [24] (and in a molecular gas, methane [25]) was successfully completed, we have now essentially concluded the field of binary collision-induced light scattering, and the measurement of the invariants of the diatomic polarizability. At the time of this writing, we are preparing to measure collision-induced scattering in ^3He , the rare isotope of helium. Next we plan to do the experiment in hydrogen (and perhaps in deuterium). Finally, mixtures of gases and the atmospheric gases will be tried. All of this will probably be completed by March 31, 1980. Thereafter, the emphasis will be on the spectroscopy of the dimer and the associated refinement of the interatomic potentials.

The superelastic electron scattering experiment is developed along two lines. On the one side we develop the electron scattering facility, and on the other side the laser system has to be set up. During the last year the electron analyzer (127° type) has been refined to 100 mV resolution with 300 eV incident energy. A sequence of beam spectra has been recorded as a function of the electron optical parameters in the gun. The search is still underway to find the combination of dimensions, which allows us to circumvent the "BOERSCH" effect, and thus to produce the most intense and monochromatic electron beam allowed by thermodynamic principles. Our second point of attention is devoted to our new argon ion pumped, mode-locked dye laser system. The laser table (5000 lb granite floating on NRC pneumatic supports) and the laser were installed in January 1979. Since then we have been building the diagnostic accessories, which cannot be purchased, and we are modifying the system to extend the spectral range of the laser systems into the 2300 Å domain. Furthermore, preliminary tests are being performed to anticipate which power and tunability can be expected in the optical pumping of the molecular jets. To this end we measured the power dependance of the doubling efficiency of several crystals. According to our preliminary

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results we can expect one watt peak power at 2300 Å, which will be enough to saturate the electronic transitions to be studied in SO₂. Furthermore, in order to measure the pulse shape of several picoseconds we are building a new type of correlator based on a rotating glass plate. A cavity dumper operating in the blue spectral range has been ordered (funded by U.T. at \$16,000), and this will further increase our doubling efficiency but requires computer controlled tuning mechanisms.

As mentioned above, with the end of the current funding period (March 31, 1980), we will have completed the work concerning the spectroscopy of binary collisions. Continued work concerns the related spectroscopy of dimers and will be proposed under this unit number.

Our work in high energy electron scattering was sponsored several years by the JSEP program. However, last year the NSF has picked up the funding of that work and the papers [26-30], are the results based largely on former data and therefore the contributions of the JSEP program has been acknowledged. There will be three or four more papers coming in the future in this area before we have taken care of all results accumulated previously. After the NSF has come in to help support our work, a new direction of research was proposed to JSEP. During the next year or two we hope to build up a new facility which centers around the studies of the electronic excited states of molecules by superelastic electron scattering. This technology will be very powerful, because it is applicable to very diversified questions ranging from air pollution to high powered lasers. In the near future our main interest will focus on small, relatively well known molecules, such as SO₂, NO₂ or J₂, where experiment and theory can meaningfully compliment each other. We have to recognize that The University of Texas at Austin has generously helped to open this new research avenue with a \$58,000 equipment grant, and a proposal for more internal money is pending.

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Research Unit QE8-3. HIGH POWER LASER SYSTEMS

Principal Investigators: Professor J. Keto (471-4151)
Professor M.F. Becker (471-3628)

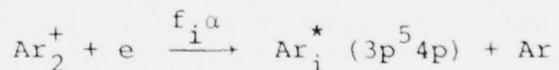
Graduate Student: C. Kuo

A. PROGRESS

1. Energy Transfer in Laser Systems. One objective of this unit is the use of time dependent spectroscopic techniques to identify the primary energy transfer processes in high-energy laser systems. Initial research has concentrated on studies of electron beam pumped mixtures of oxides and rare gases. This work is now concluded. New experiments have been directed at studies of recombination rates in high-density rare gas discharges. This information is pertinent to nearly all types of high-power excimer lasers which use rare gases as a buffer in the energy absorption process. We have now obtained very exciting preliminary data on recombination processes at high densities.

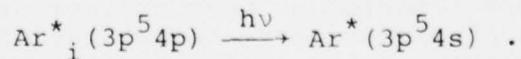
a) Recombination in High Density Argon

Biondi [1] has recently studied dissociative recombination of electrons and Ar_2^+ diatomic ions in argon discharges at 10T and shown that the argon $3p^54p$ states result from dissociative recombination



and that the decay of these states accurately follows the ion density.

For argon pressures on the order of ten atmospheres the excitation volumes are too small for reliable electron density measurements using microwave interferometry; hence we have measured the recombination rates by measuring the time dependent fluorescence of these states in the transition



If the decay is dominated by repopulation from recombination channels we expect the decay to be described by

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$$\frac{dn_i}{dt} = f_i \alpha [Ar_2^+] [ne] - \left(\sum_{j \neq i} k_{ij}^P + \sum_k k_{ik}^P + \sum_k A_{ik} \right) n_i \quad (1)$$

where f_i is the branching fraction for the recombination reaction to the i th atomic state, α is the dissociative recombination rate, n_i is the state population, n_e is the electron density, k_{ij} and k_{ik} are respectively the intramultiplet and intermultiplet collisional quenching rates, and A_{ik} is the spontaneous emission rate.

We show elsewhere [2] that if the inverse square root of the intensity is plotted as a function of time, the data should lie on a straight line with slope

$$m_i = \left(\frac{\sum_k A_{ik} + \sum_k k_{ik}^P + \sum_{j \neq i} k_{ij}^P}{A_{ik}} \right)^{\frac{1}{2}} \left(\frac{2\alpha}{f_i} \right)^{\frac{1}{2}} \quad (2)$$

and intercept

$$b_i = \frac{1}{[e]_0} \left(\frac{2}{f_i \alpha} \right)^{\frac{1}{2}} \left(\frac{\sum_k A_{ik} + \sum_k k_{ik}^P + \sum_{j \neq i} k_{ij}^P}{A_{ik}} \right)^{\frac{1}{2}} \quad (3)$$

Since recombination is a non-linear process we have measured the radiative emission rates in absolute intensity per unit volume. If we sum over all significant product states the effect of both the branching fractions and intramultiplet collision rates are eliminated, enabling the measurement of the total electron ion recombination coefficient α .

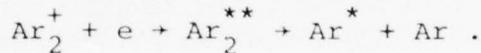
Our measurements of the decay of these states in the late afterglow confirm Biondi's observation that they are repopulated by dissociative recombination. In Fig. 1 we plot the inverse square root of the intensity for the $3p^5 4p^1 \frac{1}{2}, 1$ state observed at 826.4 nm. The same decay is observed at 696.5 nm and 712.3 nm. By measuring the slope and intercept as a function of beam current and argon pressure for all products of dissociative recombination, the branching fractions, recombination coefficients, and electron densities were determined as a function of pressure and electron density. We have obtained three significant results [2]:

- (1) The branching fraction for the $3p^5 4p^1 \frac{1}{2}, 1$ state at high densities is nearly 0.9.

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(2) The recombination coefficient at intermediate pressures (100T) is a function of electron density.

This electron density dependence of the recombination rate is not an effect of the electron temperature. The measure rates shown in Fig. 1 were obtained for time scales long with respect to 1 μ sec (5 μ sec per point). Calculations indicate that the electron distribution thermalizes in less than 1 μ sec for pressures above 100T. We believe the observed variation in recombination rate with electron density supports the idea that intermediate molecular states play an important role in dissociative recombination



This intermediate state, being near the ionization continuum, can be ionized



as well as de-excited by electron impact. Ionization processes have the effect of reducing the recombination rate, while de-excitation increases it. As a result, the recombination rate becomes dependent upon the electron density.

(3) The recombination coefficient at constant electron density is constant from 100T - 500T and then increases slowly for pressures up to 3000T. This result is shown in Fig. 2.

The observed increase in recombination rate at higher densities can be attributed to the conversion of diatomic to triatomic ions at higher densities.



Using data we are now obtaining at higher pressures, we expect to determine the recombination coefficient for Ar_3^+ .

Intermediate to our obtaining the above data we had to measure the collisional deactivation rates indicated in Eq. 1. We have studied these by observing the decay frequencies from the $\text{Ar}^*(3p^54p)$ states following electron impact excitation [3]. When using electron beam excitation, one must carefully extract possible cascade processes to

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obtain accurate measurements of the lifetimes. Unfortunately the state lifetimes and the cascade lifetimes turned out to be nearly equal; this has limited the accuracy of our measurements of the quenching time constants. However for pressures from 1T to 8T, Setser [4] has recently measured the collisional de-excitation rates for argon $3p^54p$ states produced selectively by laser excitation. Setser's data agree with ours and are more accurate because the selective excitation eliminates the effect of cascade.

Our data for the cascade decay times, shown in Fig. 3, indicates all states are populated by cascade from $\text{Ar}(3p^54p)$ states. Surprisingly, the $4p^1, 1$ state is selectively populated by cascade from an unidentified long-lived state. This result is significant because it is this state which has the large branching fraction for recombination at high density.

In addition to measuring recombination rates at higher densities we are now attempting to identify and study the intermediate states in dissociative recombination. Initial experiments have indicated we can measure the lifetime of these states. For spectroscopic identification of these states, we are planning two and three photon excitation studies of high-rydberg molecules. For this purpose we have constructed a dye laser system pumped with a high power nitrogen laser [5]. In addition we plan to repeat measurements of exciton lifetimes in solid xenon [8] using multi-photon excitation.

b) Production of $\text{O}(^1\text{S}_0)$ in Electron Beam Pumped Argon Doped with Oxygen

Previously we have reported that significant amounts of $\text{O}(^1\text{S}_0)$ are produced in electron beam pumped argon doped with oxygen. We have found from the beam current dependence that the primary production is through charge transfer



which must compete with dissociative recombination of Ar_2^+ . In calculating the $\text{O}(^1\text{S}_0)$ intensity we must account for the quenching of $\text{O}(^1\text{S}_0)$ by the dissociation products $\text{O}(^3\text{P})$ and O_3 which are produced by the discharge. We are now finishing detailed calculations for the discharge which include thirteen reaction processes. The recombination data recently obtained for argon is being used in these calculations to model the loss of argon ions. By comparing these discharge calculations with experimental data we hope to estimate the rate of charge transfer. To date we have

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obtained qualitative but not quantitative agreement with our experiments. Our data suggests an additional mechanism for O_2 dissociation is required. Results on electron dissociation of H_2 , recently obtained by Phelps [6], suggest electron dissociation of O_2 should be rapid above threshold. Since good cross sections for electron dissociation of O_2 are not available, we will have to model them with adjustable parameters. Since the only other fitted parameter is the charge transfer rate this might be done with some sensitivity. A publication on these results is in preparation [7].

2. Laser System Components. A second objective of the research in this unit is the characterization of optical components used in high power laser systems. The need for High Energy Laser beam diagnostics such as amplitude and phase distributions is well established. The grating pair or grating rhomb is frequently used in such an application. Our objective is to determine analytically the inherent aberrations in grating rhomb systems. An optimum or alternative configuration can then be developed. In addition, a deconvolution algorithm should be devised which can correct data already taken using an arbitrary rhomb system containing aberrations.

At present we have successfully analyzed the inherent aberrations in the grating rhomb beam sampler [9,10]. Although plane wavefronts are sampled without aberration, spherical or more complex wavefronts suffer one dimensional phase and displacement deviations. We have formulated an inverse filter description which employs the angular spectrum concept for the incident and sampled beams. An inverse filter is easily synthesized and may be used to deconvolute amplitude and phase data from a typical grating rhomb beam sampling system. In addition, we performed an optimization analysis in order to minimize the phase errors in the sampled beam. Some practical examples analyzed show that a phase deviation of 80 wavelengths over a curved wavefront beam can be optimized to 1/10 wavelength for the same beam. If an optimized system is used, deconvolution of the sampled beam data is seldom necessary.

Analysis and improvement of the grating rhomb beam sampler will continue during the coming year in collaboration with Dr. Jerome Knopp, MIT Lincoln Laboratory. A further publication is presently in preparation [10].

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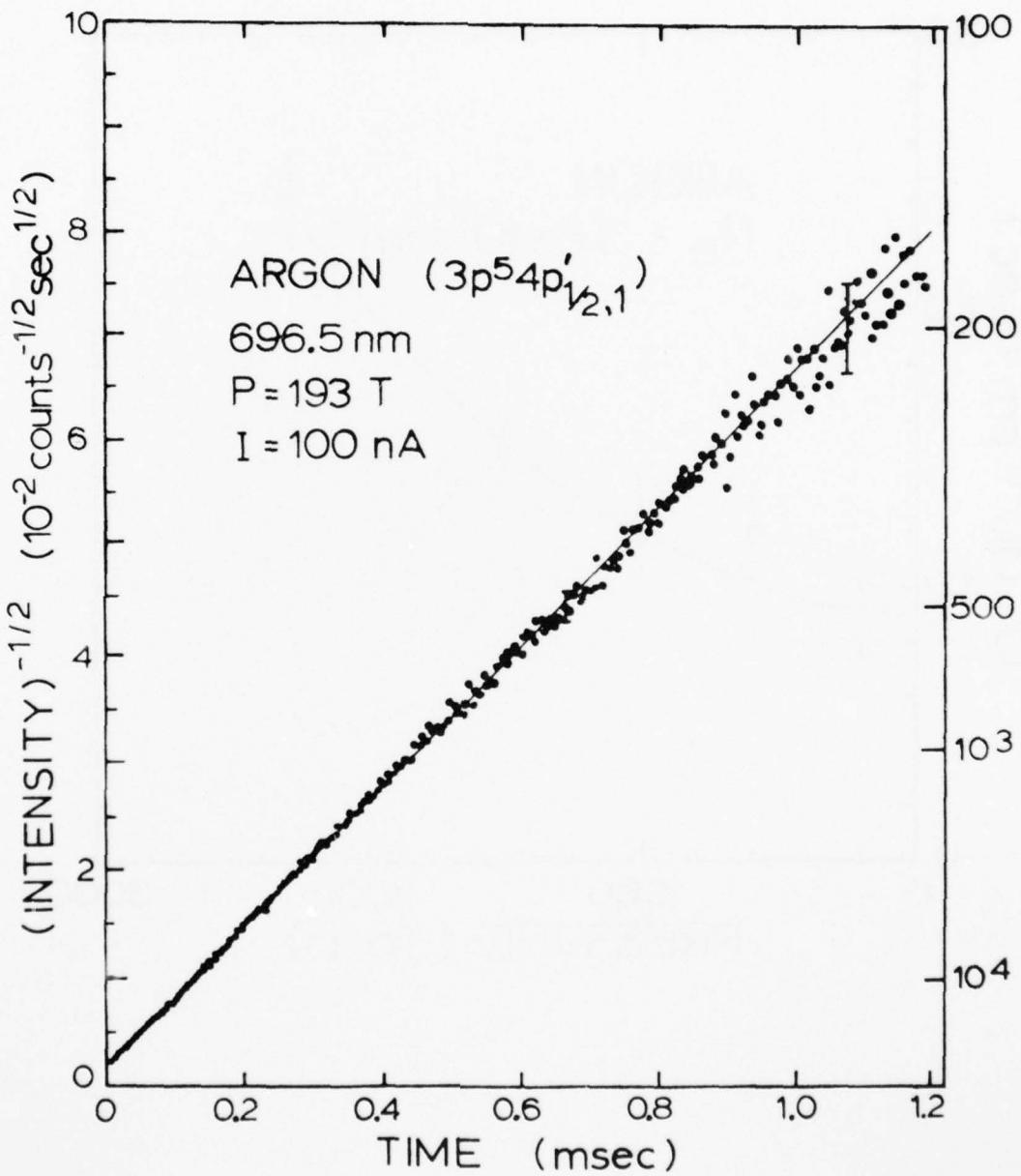


Figure 1. Inverse square root of the intensity of the argon (3p⁵, 4p'_{1/2,1} → 3p⁵, 4s_{1/2,2}) transition plotted as a function of time.

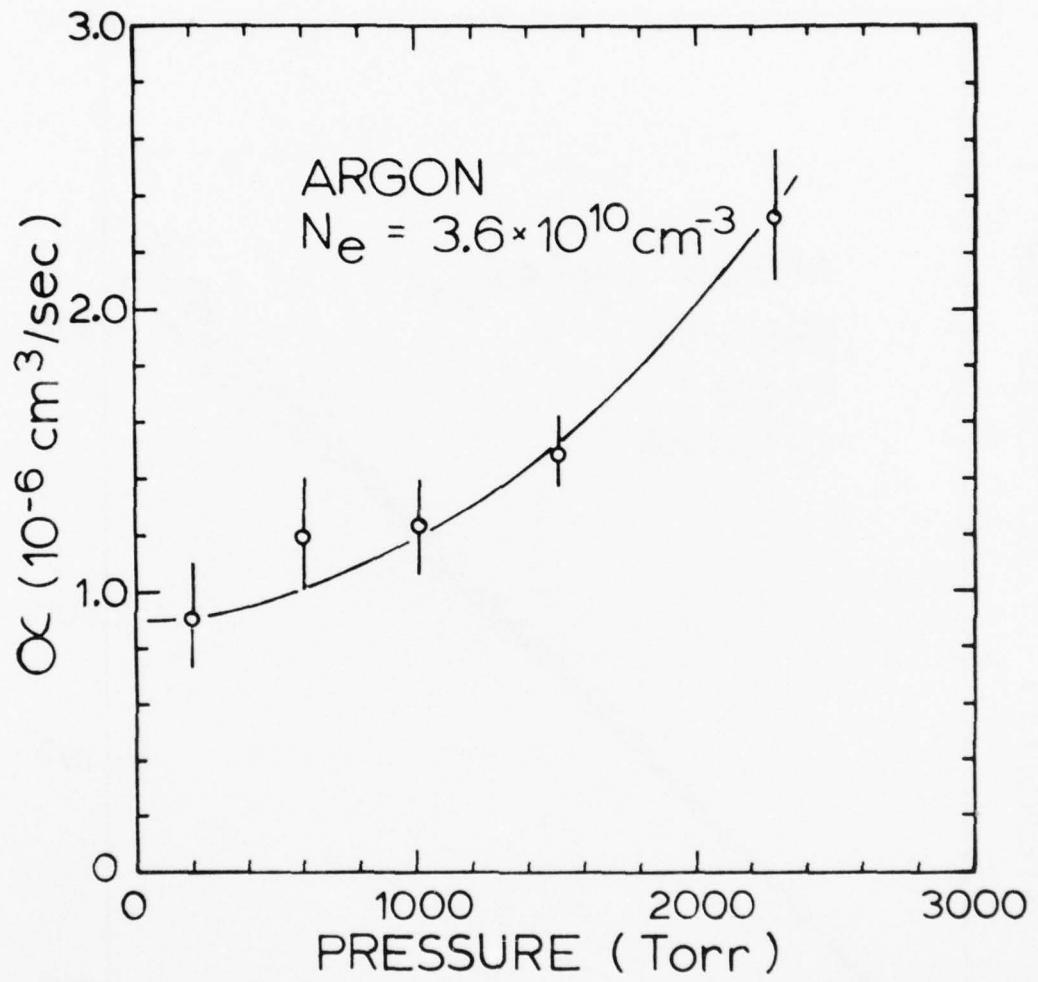


Figure 2. Recombination coefficient of ions and electrons in argon plotted as a function of pressure. The error bars shown represent relative errors.

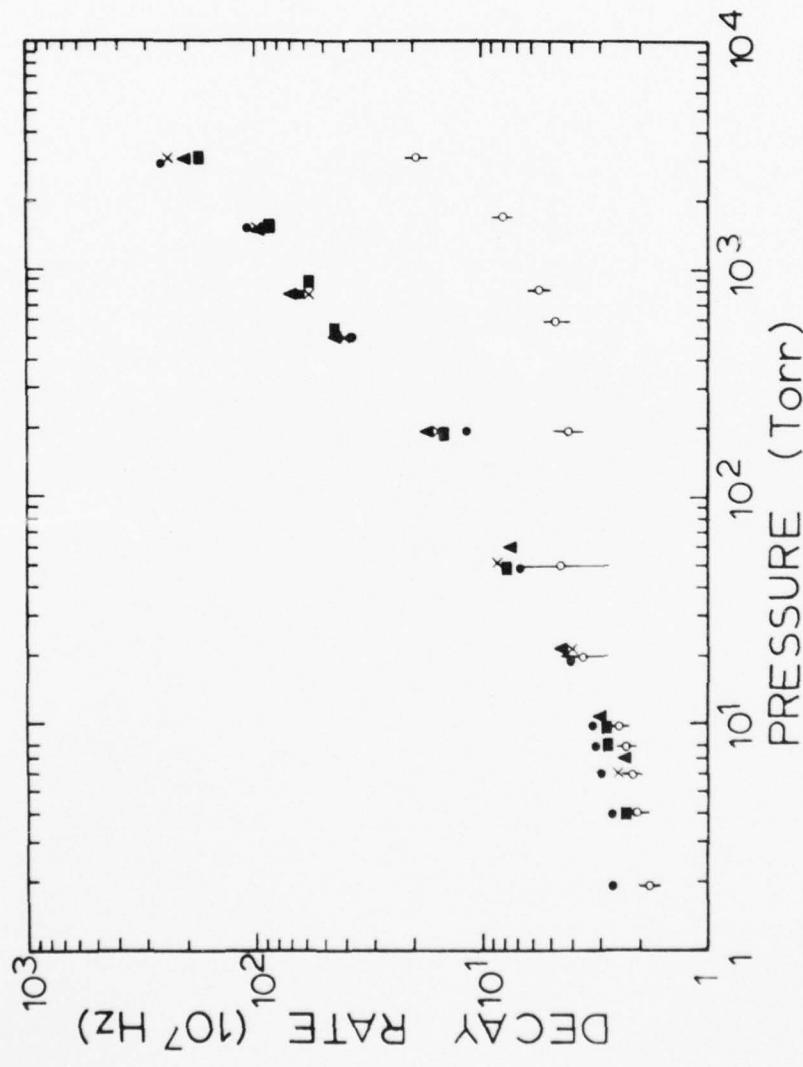


Figure 3. Decay rates for the cascade components of argon $(3p^5, 4p)$ transitions plotted as a function of argon pressure. Shown are four transitions \bullet 750.4 nm, \blacksquare 738.4 nm, \blacktriangle 751.5 nm, and \times 794.8 nm of seven which behave similarly at high pressures. The $(3p^5, 4p^{\prime}, 1 \rightarrow 3p^5, 4s^{\prime}, 2)$ state shown as open circles decays slower at higher pressures. All states decay differently at low pressures, which is characteristic of cascade from the $3p^5, 3d$ manifold.

RESEARCH GRANTS AND CONTRACTS

FEDERAL FUNDS

U.S. Air Force Office of Scientific Research, AFOSR 77-3190, "Automatic Recognition and Tracking of Objects," Professor J.K. Aggarwal, Principal Investigator, December 1, 1976 - November 30, 1978.

U.S. Air Force Office of Scientific Research, AFOSR 77-3409, "An Integrated Methodology and Tools for Software Development," Profs. Yeh, Chandy and Chester, Principal Investigators, July 1, 1978 - June 30, 1979.

U.S. Air Force Office of Scientific Research, AFOSR 79-0025, "Optimal and Suboptimal Estimation for Nonlinear Stochastic Systems," Professor S.I. Marcus, Principal Investigator, December 1, 1978 - November 30, 1979.

U.S. Air Force Office of Scientific Research, AFOSR 77-3385, "The Study of Nonparametric Procedures for Discrimination and Clustering Problems," Professor T.J. Wagner, Principal Investigator, July 1, 1977 - July 31, 1979.

U.S. Air Force Office of Scientific Research, AFOSR 76-3062, "Bivariate Distributions and Their Applications in Communication Theory," Professor Gary L. Wise, Principal Investigator, June 15, 1976 - June 30, 1979.

U.S. Air Force Office of Scientific Research, AFOSR 76-3062, "The Study of Certain Statistical Aspects of Discrimination, Clustering, and Communication Theory," Professor Gary L. Wise, and Professor Terry J. Wagner, Co-Principal Investigators, July 1, 1979 - September 30, 1980.

U.S. Air Force Office of Scientific Research, AFOSR 78-3712, "New Nonlinear Optical Processes in Molecules at Infrared Frequencies," Professor M.F. Becker, Principal Investigator, October 1, 1978 - September 30, 1980.

U.S. Army Research Office, DAAG29-78-G-0146, "Quasi-optical Techniques for Millimeter and Submillimeter-wave Circuits," Professor T. Itoh, Principal Investigator, July 1, 1978 - October 31, 1980.

U.S. Army Research Office, DAFG 60-78-C-0161, "Data Processing Requirements - Modelling Technology," Professor R.T. Yeh, Principal Investigator, October 1, 1978 - September 30, 1979.

Office of Naval Research Contract N00014-75-C-0916, Mod. P0003, "Acquisition of Dedicated SEM with Option for TED," Professors R.W. Bene' and R.M. Walser, Principal Investigators, May 1, 1977 - April 30, 1978.

RESEARCH GRANTS AND CONTRACTS

Office of Naval Research Contract N00014-75-C-0753, "Multiple and/or Inhomogeneous Layers for Integrated Optical Coupling and Modulation," Professor A.B. Buckman, Principal Investigator, March 1, 1978 - February 29, 1980.

Office of Naval Research Contract N00014-75-C-0916, "Synthesis of Useful Electronic Structures Using Solid-Solid Phase Reactions Near Surfaces," Professors R.W. Bene' and R.M. Walser, Principal Investigators, May 1, 1975 - April 30, 1979.

National Aeronautics and Space Administration, Lewis Research Center Grant NSG 3089, "Development of a Plasma Fluctuation Diagnostic Tool for the NASA Lewis Bumpy Torus Experiment," Professor E.J. Powers, Principal Investigator, November 15, 1975 - December 31, 1978.

National Science Foundation, MCS 78-07306, "Computer Science and Computer Engineering Research Equipment," Professor R.T. Yeh, Principal Investigator, June 15, 1978 - November 30, 1979.

National Science Foundation, CHE 77-21548, "Experimental Termination of Charge Densities by Electron Diffusion," Professor M. Fink, Principal Investigator, February 15, 1978 through February 15, 1980.

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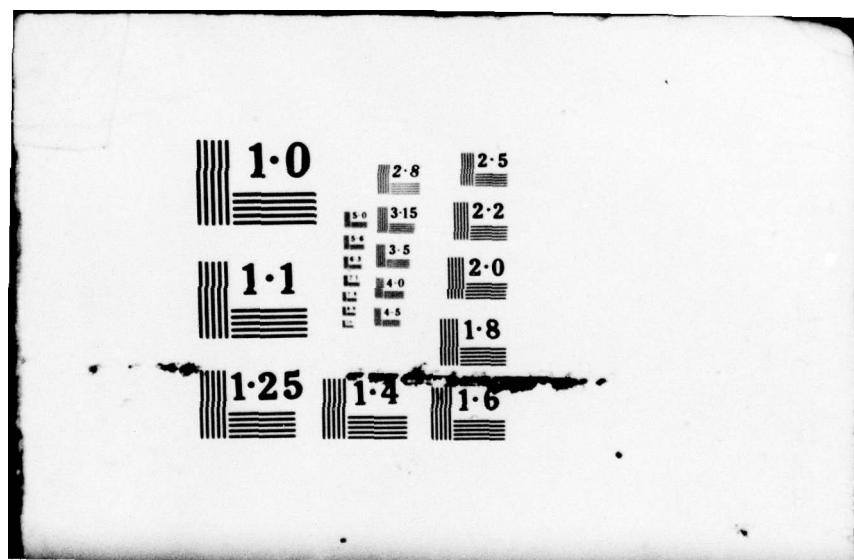
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Department of Defense Joint Services Electronics Program Research Contract F49620-77-C-0101, "Basic Research in Electronics," Professor E.J. Powers, Principal Investigator on behalf of the Faculty Affiliates of the Electronics Research Center, April 1, 1978 - March 31, 1979.

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Bureau of Engineering Research, "Control Issues in Distributed Computer Systems," Professor T.K.M. Agerwala, Principal Investigator, September 1, 1978 - August 31, 1979.

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State of Texas Center for Energy Studies, "Electric Vehicle Project," Professor B.F. Womack, Principal Investigator, September 1, 1977 - August 31, 1978.

Texas Atomic Energy Research Foundation, "Analysis and Interpretation of Plasma Fluctuation Data Utilizing Digital Time Series Analysis," Professor E.J. Powers, Principal Investigator, May 1, 1977 - April 30, 1980.

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